
 Substitute Form PTO-1449  
(Modified)

 U.S. Department of Commerce  
Patent and Trademark Office

 Attorney's Docket No.  
06618-607002

 Application No.  
10/010,725

**Information Disclosure Statement  
by Applicant**

(Use several sheets if necessary)

(37 CFR §1.98(b))

Applicant

 Wely B. Floriano, Nagarajan Vaidehi, William A.  
Goddard, III

Filing Date

November 30, 2001

Group Art Unit

1645

**U.S. Patent Documents**

Examiner Initial	Desig. ID	Patent Number	Issue Date	Patentee	Class	Subclass	Filing Date If Appropriate
PW	AA	5,680,319	10/21/97	Rose et al.	364	496	
PW	AB	5,705,335	1/6/98	Hendry	435	6	
PW	AC	5,873,052	2/16/99	Sharaf	702	20	
PW	AD	5,854,992	12/29/98	Shakhnovich et al.	702	27	
PW	AE	5,940,307	8/17/99	Fischbarg et al.	364	496	

**Foreign Patent Documents or Published Foreign Patent Applications**

Examiner Initial	Desig. ID	Document Number	Publication Date	Country or Patent Office	Class	Subclass	Translation	
							Yes	No
	AF							

**Other Documents (include Author, Title, Date, and Place of Publication)**

Examiner Initial	Desig. ID	Document
PW	AG	D'Aquino, J. et al., "The Magnitude of the Backbone Conformational Entropy Change in Protein Folding," <u>Proteins: Structure, Function and Genetics</u> (1996) 25:143-156
	AH	Buck, L. et al., "A Novel Multigene Family May Encode Odorant Receptors: A Molecular Basis for Odor Recognition," <u>Cell</u> (1991) 65:175-187
	AI	Burkhard, P. et al., "An Example of a Protein Ligand Found by Database Mining: Description of the Docking Method and Its Verification by a 2.3 Å X-ray Structure of a Thrombin-Ligand Complex," <u>J. Mol. Biol.</u> (1998) 277:449-466
	AJ	Connolly, M.L., "Solvent-Accessible Surfaces of Proteins and nucleic Acids," <u>Science</u> (1983) 221(4612):709-713
	AK	Ding, H. Q. et al., "Atomic Level Simulations on a Million Particles: The Cell Multipole Method for Coulomb and London Nonbond Interactions", <u>J. Chem. Phys.</u> (1992) 97(6):4309-4315
	AL	Datta, D. et al, "Mechanism for Antibody Catalysis of the Oxidation of Water by Singlet Dioxide", <u>PNAS</u> (2002) 99(5):2636-2641
	AM	Ding, H.Q. et al. "The Reduced Cell Multipole Method for Coulomb Interactions in Periodic Systems with Million-Atom Unit Cells", <u>Chem. Phys. Lett.</u> (1992) 196 (1,2):6-10
	AN	Dombi, G. et al., "Analysis of Protein Transmembrane Helical Regions by a Neural Network", <u>Protein Science</u> (1994) 3:557-566
	AO	Donnelly, D. "Modeling alpha-helical Transmembrane Domains", <u>Biochem. Society Transactions</u> (1993) 21:36-39
	AP	Ewing, T.A. et al., "Critical Evaluation of Search Algorithms for Automated Molecular Docking and Database Screening", <u>J. Comput. Chem.</u> (1997) 18:1175-1189
	AQ	Floriano, W. B. et al., "Molecular mechanisms underlying differential odor responses of a mouse olfactory receptor", <u>PNAS</u> (2002) 97(20):10712-10716
	AR	Gasteiger, J. et al., "Iterative Partial Equalization of Orbital Electronegativity - a Rapid Access to Atomic Charges", <u>Tetrahedron</u> (1980) 36:3219-3288

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PW	AS	Ghosh, A. et al., "Generalized born model based on a surface integral formulation", <u>J. Phys. Chem.</u> (1998) 102:10983-10990
	AT	Guner, O., <u>Pharmacophore - Perception, Development and Use in Drug Design</u> (2000)
	AU	Huang, E. et al., "Ab Initio Fold Prediction of Small Helical Proteins Using Distance Geometry and Knowledge-Based Scoring Functions", <u>Journal of Molecular Biology</u> (1999) 290:267-281
	AV	Jain, A., et al., "A fast recursive algorithm for molecular-dynamics simulation", <u>J. Comp. Phys.</u> (1993) 106:258-268
	AW	Juretic, D. et al., "Conformational Preference Functions for Predicting Helices in Membrane Proteins", <u>Biopolymers</u> (1993) 33:255-273
	AX	Kiyama, R. et al., "Homology Modeling of Gelatinase Catalytic Domains and Docking Simulations of Novel Sulfonamide Inhibitors" <u>Journal of Medicinal Chemistry</u> (1999) 42:1723-1738
	AY	Krautwurst, D. et al., "Identification of Ligands for Olfactory Receptors by Functional Expression of a Receptor Library", <u>Cell</u> (1998) 95:917-926
	AZ	Kuntz, I. et al., "A Geometric Approach to Macromolecule-Ligand Interactions," <u>J. Mol. Biol.</u> (1982) 161:269-288
	AAA	Lim, K. et al., "Molecular Dynamics for Very Large Systems on Massively Parallel Computers: The MPSim Program", <u>J. Comput. Chem.</u> (1997) 18:501-521
	ABB	Malnic, B. et al., "Combinatorial Receptor Codes for Odors", <u>Cell</u> (1999) 96: 713-723
	ACC	Mathiowetz, A.M. et al., "Protein Simulations using Techniques Suitable for Very Large Systems: the Cell Multipole Method for Nonbond Interactions and the Newton-Euler Inverse Mass Operator Method for Internal Coordinate Dynamics", <u>Proteins: Structure, Function, and Genetics</u> (1994) 20:227-247
	ADD	Mayo, S. L. et al. "DREIDING - a generic force field for molecular simulations", <u>J. Phys. Chem.</u> (1990) 94:8897-8909
	AEE	McCammon, J. and Harvey, S.C., <u>Dynamics of Proteins and Nucleic Acids</u> (1987)
	AFF	McMartin, C. et al., "QXP: Powerful, Rapid Computer Algorithms for Structure-Based Drug Design", (1997) 11:333-344
	AGG	Mombaerts, P., "Seven-Transmembrane Proteins as Odorant and Chemosensory Receptors", <u>Science</u> (1999) 286:707-711
	AHH	Morris, G.M. et al., "Automated Docking Using a Lamarckian Genetic Algorithm and an Empirical Binding Free Energy Function" <u>J. Comp. Chem.</u> (1998) 19(14):1639-1662
	AII	Palczewski, K., et al., "Crystal Structure of Rhodopsin: A G Protein-Coupled Receptor," <u>Science</u> (2000) 289:739-745
	AJJ	Pilpel, Y. et al. "The variable and conserved interfaces of modeled olfactory receptor proteins" <u>Prot. Sci.</u> (1999) 8:969-977
	AKK	Poincelot, R., et al., "Determination of the Chromophoric Binding Site in Native Bovine Rhodopsin," <u>Biochemistry</u> (1970) 9(8):1809-1816
	ALL	Rappé, A.K. et al., "Charge Equilibration for Molecular Dynamics Simulations", <u>J. Phys. Chem.</u> (1991) 95:3358-3363
	AMM	Reshetnikova, L. et al., "Crystal Structures of Phenylalanyl-tRNA Synthetase Complexed with Phenylalanine and a Phenylalanyl-adenylate Analogue", <u>J. Mol. Biol.</u> (1999) 287:555-568

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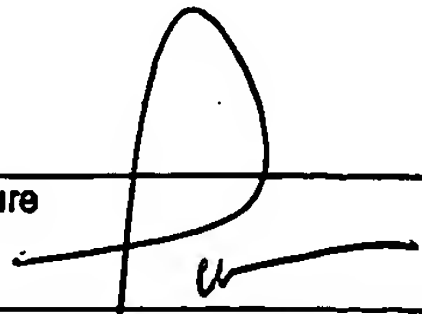
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PW	ANN	Sachdeva, A. et al., "Nasal Mucociliary Clearance & Mucus pH in patients with Diabetes Mellitus," <u>Indian J. Med. Res.</u> (1993) 98:265-268
	AOO	Sansom, M. et al., "Modeling Transmembrane Helix Bundles by Restrained MD Simulations", Chapter 14 (pp. 325-347), In Webster, D., <u>Protein Structure Prediction: Methods and Protocols</u> (2000)
	APP	Schertler, G.F.X., "Structure of rhodopsin", <u>Eye</u> (1998) 12:504-510
	AQQ	Sharma N., et al., "Efficient introduction of aryl bromide functionality into proteins in vivo", <u>FEBS Lett.</u> (2000) 467:37-40
	ARR	Shoichet B.K. et al., "Ligand Solvation in Molecular Docking", <u>Proteins: Structure, Function and Genetics</u> (1999) 34:4-16
	ASS	Schoichet, B.K. et al., "Structure-Based Discovery of Inhibitors of Thymidylate Synthase," <u>Science</u> (1993) 259:1445-1450
	ATT	Singer, M. et al., "Molecular Modeling of Ligand-Receptor Interactions in the OR5 Olfactory Receptor", (1994) <u>Neuroreport</u> 5:1297-1300
	AUU	Singer, M.S., "Analysis of the Molecular Basis for Octanal Interactions in the Expressed Rat 17 Olfactory Receptor," <u>Chem. Senses</u> (2000) 25:155-165
	AVV	Singer, M.S. et al. "Positive Selection Moments Identify Potential Functional Residues in Human Olfactory Receptors", <u>Receptors and Channels</u> (1996) 4:141-147
	AWW	Tannor, D. et al. "Accurate First Principles Calculation of Molecular Charge Distributions and Solvation Energies from Ab Initio Quantum Mechanics and Continuum Dielectric Theory", <u>J. Am. Chem. Soc.</u> (1994) 116:11875-11882
	AXX	Uechi et al., "An Automated Structure Prediction System by Lattice Model for Seven-Helix-Type Membrane Proteins", <u>Genome Informatics</u> (1999) 10:239-240
	AYY	Vaidehi, N. et al., "Prediction of Structure and Function of G Protein-Coupled Receptors", <u>PNAS</u> (2002) 99:12622-12627
	AZZ	Vaidehi, N. et al. "Constant Temperature Constrained Molecular Dynamics: The Newton-Euler Inverse Mass Operator Method", <u>J. Phys. Chem.</u> (1996) 100:10508-10517
	AAAA	Vriend, G., "WHAT IF: a molecular modeling and drug design program", <u>J. Mol. Graph.</u> (1990) 8:52-56
	ABBB	Williams, R.L., et al., "Empirical Solvation Models in the Context of Conformational Energy Searches: Application to Bovine Pancreatic Trypsin Inhibitor," <u>Proteins: Structure, Function, and Genetics</u> (1992) 14:110-119
	ACCC	Zou, X., et al., "Inclusion of Solvation in Ligand Binding Free Energy Calculations Using the Generalized-Born Model," <u>J. Am. Chem. Soc.</u> (1999) 121:8033-8043
	ADDD	Floriano, W.B. et al., "Design of Lead Antagonists for Transcriptional Regulation of Glucocorticoid Responsive Elements," U.S. Provisional Application No. 60/233,294, filed 09/15/00

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